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# A comparison of the performance of profile position and composition estimators for quality control in binary distillation

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## Abstract

In this study a number of control strategies have been developed for control of the overhead composition of a binary distillation column. The nonlinear wave model as presented in the literature, has been substantially modified in order to express it in variables that can easily be measured and make it more robust to feed flow and feed composition changes. The new model consists essentially of the equation for wave propagation and a static mass and energy balance across the top section of the column. Taylor series developments are used to relate the temperature on the measurement tray to the temperature and concentration on the tray where the inflection point of the concentration profile is located. The model has been incorporated in control of the overhead quality of a toluene/*o*-xylene benchmark column. In addition, a number of partial least squares (PLS) estimators have been developed: a nonlinear estimator for inferring the overhead composition from temperature measurements and a linear and nonlinear estimator for inferring the inflection point of the concentration profile in the column. These estimators are also used in a cascade control strategy and compared with use of the wave propagation model. Finally a control strategy consisting of a simple temperature controller and a composition controller were implemented on the simulated column. The study shows that the inferential control using PLS estimators performs equally well than control using the nonlinear wave model. In all cases the advantage of using inferential controllers is substantial compared with using single tray temperature control or composition control.

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**Keywords:** Binary distillation; Partial least squares; Wave propagation model

## 1. Introduction

Systems with distributed parameters, such as distillation columns, exhibit dynamic characteristics that resemble traveling waves (Luyben, 1972; Marquardt, 1986; Hwang, 1991, 1995).

Luyben (1972) pioneered a temperature profile position controller by measuring the temperature on five trays and calculating ‘between which trays a temperature in the middle of break lies’. This control strategy exhibited an increased sensitivity to feed changes. Marquardt (1986) analyzed the behavior of binary distillation columns by showing that a relationship exists between the product composition and the inflec-

tion point of the temperature profile. The idea behind the use of a profile for composition control is the fact that the shape of the profile does not necessarily have to be the same in order to guarantee a constant top (and/or bottom) composition, it only requires conformity of the profile.

Betlem (2000) has also shown experimentally that in batch columns the inflection point under constant top quality control remains constant despite the fact that the bottom composition changes continually and consequently, the dominant first order time constant remains the same.

Hwang (1991, 1995) gave a comprehensive discussion on how the shift in sharp concentration profiles in a distillation column can be explained by nonlinear wave theory.

The nonlinear wave model can be a very helpful tool for the implementation of dual composition control since it provides a fast method to infer the response of

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**Nomenclature**

$A$	constant in Antoine equation
$B$	constant in Antoine equation
$D$	molar distillate flow
$dy/dx$	derivative of vapor–liquid equilibrium relationship
$F$	molar feed flow rate
$H$	molar enthalpy
$K$	ratio between partial component pressure and system pressure
$L$	molar liquid flow rate
$M$	molar holdup
$N$	total number of trays
$p$	Pressure
$q$	vapor fraction of the feed
$Q$	heat released in the condensor
$r$	ratio between molar vapor and liquid holdup
$S$	dimensionless spatial coordinate
$t$	time or score
$T$	temperature
$u$	wave propagation velocity
$V$	molar vapor flow
$x$	mole fraction light component
$y$	vapor fraction light component
$z$	feed fraction light component
$\Delta$	difference between two sides of shock wave
<i>Subscripts</i>	
LD	liquid distillate
LS	liquid on representative tray
m	measurement
S	spatial coordinate of representative tray
VS	vapor flow on representative tray

product compositions to feed composition and feed flow changes. It is, therefore, not surprising that various control applications have been reported in the literature (Gilles & Retzbach, 1980, 1983; Balasubramhanya & Doyle, 1997, 2000; Han & Park, 1993; Shin, Seo, Han & Park, 2000). The latter two authors implement the nonlinear wave model in a dual composition Generic Model Control framework. In all cases the authors report that the control strategy based on the nonlinear wave model outperforms all other tested control strategies.

Another interesting approach to control the top and/or bottom composition in distillation columns is the use of a Partial Least Squares estimator for composition control (Mejdell & Skogestad, 1991; Kano, Miyazaki, Hasebe & Hashimoto, 2000).

Mejdell proposed three estimators for the composition, (i) an estimator using 12 weighted column temperatures, (ii) an estimator using logarithmic transformation of the composition and no weighting on the temperatures and (iii) an estimator using logarithmic transformations on temperatures and composition. Kano et al. carried out a comprehensive study

of dynamic Partial Least Squares (PLS) for composition estimation and concluded that the estimation of column top and bottom quality should be based on reflux flow rate, reboiler heat duty, pressure and multiple tray temperatures. The cascade control system studied consisted of inner temperature control loops and outer inferential composition control loops. No feedback on actual composition was, however, included in the control strategy.

In this study the nonlinear wave model will be revisited, the model is formulated such that it is dependent on easily measurable variables. The problem of maintaining a constant inflection point of the concentration profile is reduced to proper estimation of the vapor and liquid flow and of the concentration and temperature on the tray, where the inflection point of the concentration profile is located. It will be shown that several, relatively simple models can be developed to accomplish estimation of concentration and temperature. In addition, it will be shown that using the nonlinear wave model in a cascade composition control structure provides the advantage of fast response of the controlled variable.

Two PLS models will be developed in this study, one for estimation of the inflection point of the concentration profile and one for the actual overhead column composition. The use of these inferential models in a cascade control structure will also be tested and compared with the use of the nonlinear wave model. In all cases the cascade control structure uses the actual measured concentration with a 10 min dead time as the actual feedback in order to avoid any offset in the controlled composition.

## 2. Steady state column design and response to disturbances

Luyben (1990) describes a detailed dynamic model of a toluene/*o*-xylene distillation column.

Table 1 gives a summary of the steady state situation at which this column is operated. Most of the design parameters are taken from this detailed model, although some parameters are slightly different, they are summarized in Table 1.

This detailed model was taken as a reference for actual process behavior. Figs. 1 and 2 show the steady state concentration profiles of an uncontrolled column. Since the feed to the column is on temperature control, the most important disturbances that will enter the column are changes in the feed flow rate and the feed composition. The position of the so-called representa-

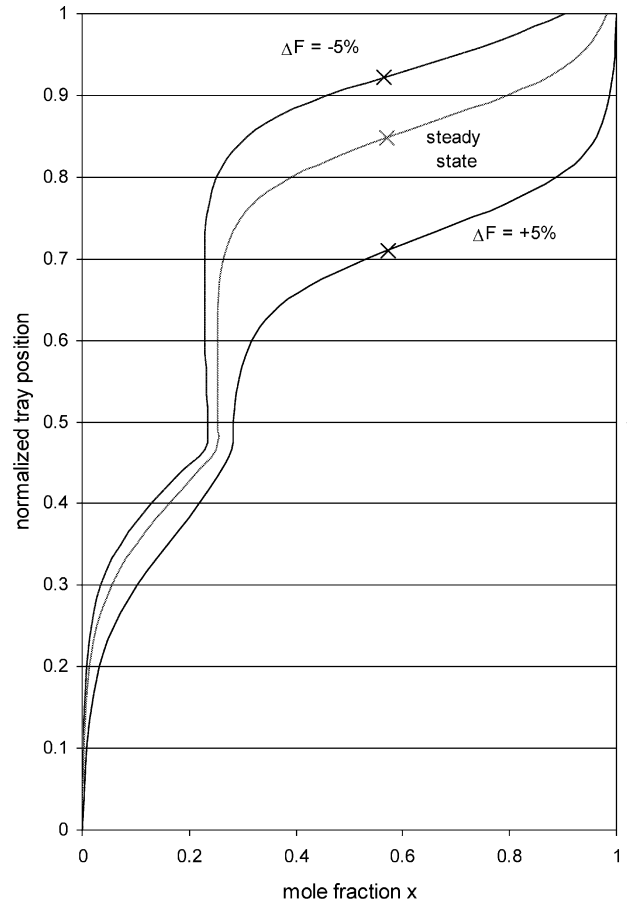


Fig. 1. Concentration profile in distillation tower for different feed rates.

tive tray (the tray where the inflection point of the concentration profile is located) is marked with an 'x'. It can be seen that this position shifts considerably with changing process conditions. In a column that is on temperature or composition control, this shift will be much less.

## 3. The nonlinear wave model

The partial mass balance for a tray of a distillation column can be written as (Hwang & Helfferich, 1988; Marquardt & Amrehn, 1994):

$$M_V \frac{\partial y}{\partial t} + M_L \frac{\partial x}{\partial t} = L \frac{\partial x}{\partial z} - V \frac{\partial y}{\partial z}, \quad (1)$$

$$z \in (0, l), \quad x(l, t) = x_l(t), \quad y(0, t) = y_0(t)$$

where  $x$  is the mole fraction of the more volatile component in the liquid,  $y$  is the mole fraction of the more volatile component in the vapor,  $M_V$  and  $M_L$  are the vapor and liquid hold-up, respectively, which are assumed to be constant,  $L$  and  $V$  are the liquid and vapor flow. Eq. (1) can be rewritten to the well-known

Table 1  
Design parameters for detailed model toluene/*o*-xylene column

Feed rate	18.0 kmol/min
Feed composition	0.33 mol fraction toluene
Cooling water flow	1.706 m <sup>3</sup> /min
Pressure in top of column	90 mmHg
Pressure in bottom of column	232.88 mmHg
UA	2.0E+4 kJ/(min °C)
Reboiler duty	6.37E+5 kJ/min
Distillate flow rate	5.97 kmol/min
Bottom flow rate	12.03 kmol/min
Reflux flow rate	10.95 kmol/min
Distillate flow composition	0.99469 mol fraction toluene
Bottom flow composition	0.00531 mol fraction toluene
Average tray liquid hold-up	7.07 kmol
Tray 27 vapor flow rate	16.11 kmol/min
Tray 27 liquid flow rate	9.90 kmol/min
Feed temperature	95.0 °C
Top temperature	49.5 °C
Bottom temperature	104.4 °C
Total number of trays	30
Feed tray location	14
Weir height	0.0612 m
Weir length	3.78 m
Dry hole pressure drop	0.134 mmHg/(kmol/m <sup>3</sup> ) per (m/s) <sup>2</sup>
Hold-up reflux drum	64.47 kmol
Hold-up column base	88.82 kmol
Vapor fraction feed	20%

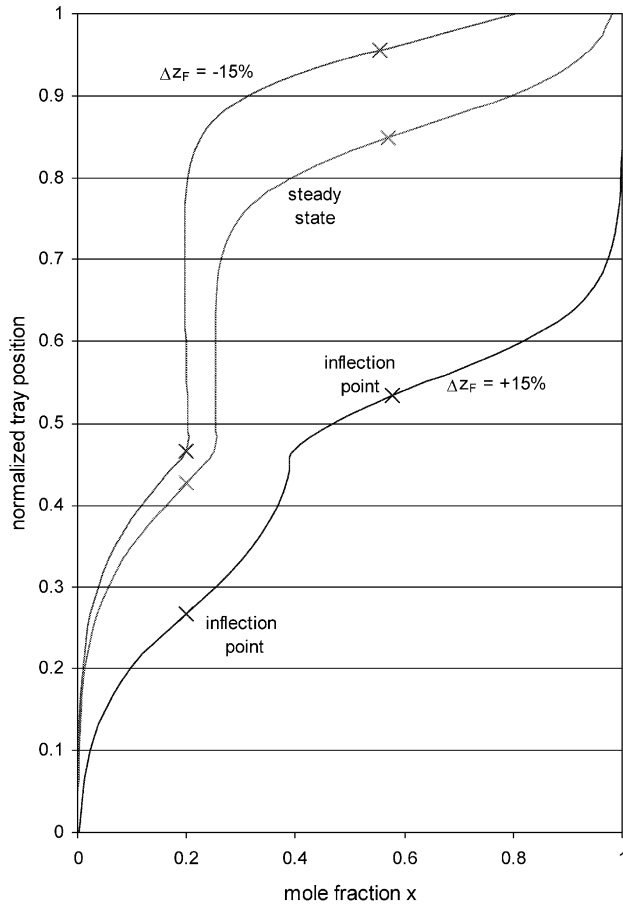


Fig. 2. Concentration profile in distillation tower for different feed compositions.

wave velocity equation for tracking the propagation of a specific value of the concentration (Hwang, 1991; Han & Park, 1993):

$$u = \frac{dS}{dt} = \frac{V}{NM_L} \frac{(dy/dx) - (L/V)}{1 + r(dy/dx)} \quad (2)$$

in which  $r = M_V/M_L$  and  $dy/dx$  is the slope of the equilibrium relationship at the specific value of the concentration and  $S$  is the spatial coordinate where the concentration profile shows an inflection point.

The wave velocity  $u$  varies with the concentration and consequently varies with location within the wave. A wave tends to sharpen if  $u$  decreases with location and such a wave is called shock wave. The velocity of this wave, in analogy of Eq. (2), can be written as (Han & Park, 1993):

$$u_{\Delta} = \left( \frac{dS}{dt} \right)_{\Delta} = \frac{V}{NM_L} \frac{(\Delta y/\Delta x) - (L/V)}{1 + r(\Delta y/\Delta x)} \quad (3)$$

where  $\Delta$  indicates the difference between the two sides of the shock wave.

In control applications this non-linear wave model is often used to ensure that the wave propagation velocity

$u_{\Delta}$  remains zero, subsequently there will be conformity in profile position, i.e. the inflection point remains unchanged. It is, therefore, important that  $\Delta y/\Delta x$  and  $L$  and  $V$  are estimated properly at the tray position where the propagation velocity is zero.

A good estimate of  $L$  and  $V$  can be obtained from a static enthalpy and mass balance across the top section of the distillation column, as shown in Fig. 3.

For small values of  $\Delta y$  and  $\Delta x$  which is the case when the process is under control, the static enthalpy balance can be written as:

$$VH_{VS} - LH_{LS} - Q_{TOP} - DH_{LD} = 0 \quad (4)$$

where  $H_{VS}$  and  $H_{LS}$  are the vapor and liquid enthalpy, respectively, at the representative tray  $S$ ,  $Q_{TOP}$  is the heat removed by the cooling water and  $H_{LD}$  is the liquid enthalpy of the distillate flow,  $D$  is the molar distillate flow.

$Q_{top}$  can be estimated from the cooling water flow rate and the water inlet and outlet temperatures.

The static mass balance for the top section of the column can be written as:

$$V - L - D = 0 \quad (5)$$

The liquid and vapor enthalpy on the representative tray can be calculated (Luyben, 1990), when the liquid and vapor compositions and the temperature on the representative tray are available.

In order to relate vapor composition to liquid composition, the concept of constant relative volatility is assumed, in which case:

$$y_S = \frac{\alpha x_S}{1 + (\alpha - 1)x_S} \quad (6)$$

where  $\alpha$  is the relative volatility ( $= 3$  in this investigation).

An estimate for the expression for  $\Delta y/\Delta x$  can be derived from this equation:

$$\frac{\Delta y}{\Delta x} \approx \frac{\alpha}{[1 + (\alpha - 1)x_S]^2} \quad (7)$$

In an actual situation, one or two temperatures close to the representative tray are measured. From simulations with the detailed process model it was found that the representative tray is close to tray 25, depending on the disturbances that act upon the process.

If the temperature measurement is called  $T_m$ , then the temperature  $T_s$  can be calculated from a first order Taylor series expansion:

$$T_s = T_m + \left( \frac{\partial T}{\partial S} \right)_m (S - S_m) \quad (8)$$

where  $S$  is the desired normalized tray position where the concentration profile shows an inflection point, and  $S_m$  is the normalized tray position of the measurement

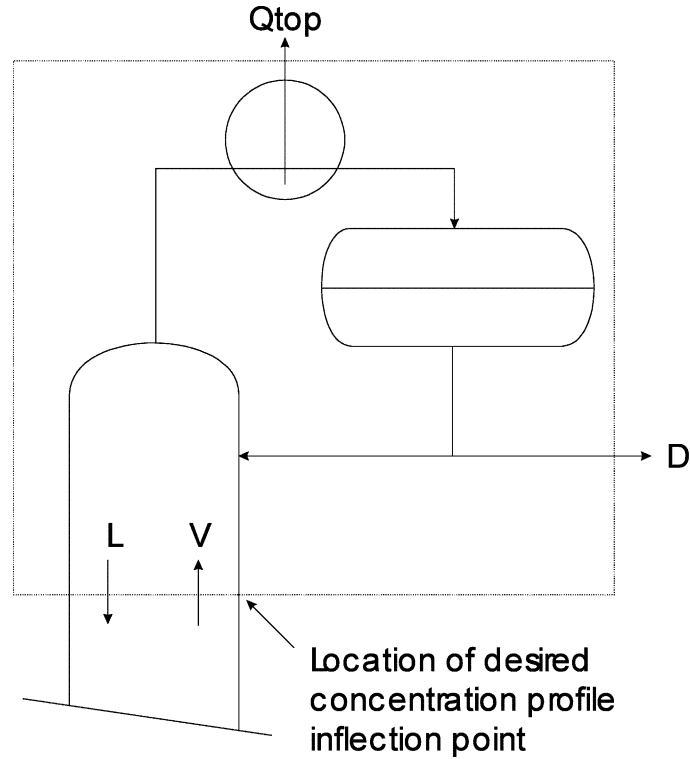


Fig. 3. Liquid and vapor flow estimation for top section of the column.

tray. The following alternatives exist for calculating the derivative  $(\partial T/\partial S)_m$  at the measurement tray:

- Assume the value is constant, take the average from simulations with the detailed model. It was found that this simple method does not provide good estimates of  $T_S$ , thus it will not be explored further.
- Assume two temperatures are measured, for example,  $T_m$  and  $T_{m+1}$ , then the derivative can be calculated from:

$$\left(\frac{\partial T}{\partial S}\right)_m = \frac{T_{m+1} - T_m}{S_{m+1} - S_m} \quad (8a)$$

If the temperature measurement is noisy then an appropriate data smoothing technique should be applied.

When only one temperature measurement is available, one could also use the following model to calculate the tray temperature  $T_S$ :

$$T_S = T_{S,\text{ref}} + \left(\frac{\partial T_S}{\partial T_m}\right)(T_m - T_{m,\text{ref}}) \quad (9)$$

in which the derivative is assumed to be constant. The derivative in Eq. (9) as well as the reference values  $T_{S,\text{ref}}$  and  $T_{m,\text{ref}}$  are obtained from simulations with a detailed tray to tray model.

The values for the constants in Eqs. (8) and (9) are given in Table 2.

Table 2  
Values of constants in Eqs. (8) and (9)

$(\partial T/\partial S)_m$ if assumed constant	−142.544 °C
$T_{S,\text{ref}}$	65.912 °C
$(\partial T_S/\partial T_m)$	0.750
$T_{m,\text{ref}}$	68.010 °C
$S$	0.84806
$S_m$	0.83333

The value of  $x_S$  can be calculated in a number of different ways. One method is to calculate the composition on the measurement tray  $x_m$  first. This can be done by the following equation:

$$x_m = x_{m,\text{ref}} + \left(\frac{\partial x}{\partial T}\right)_m (T_m - T_{m,\text{ref}}) \quad (10)$$

where the derivative follows from detailed tray to tray simulations.

Another method is to calculate  $x_m$  from phase equilibrium considerations for binary systems:

$$\sum K(i)x_m(i) = 1.0$$

$$\sum x_m(i) = 1.0 \quad (11)$$

The variable  $K(i)$  can be calculated from:



$$p(i) = \exp\left(\frac{A(i)}{T_m} + B(i)\right)$$

$$K(i) = \frac{p(i)}{p_m} \quad (11a)$$

where  $p_m$  is the pressure at the measurement tray,  $p(i)$  is the partial component pressure; A and B are component constants and  $T_m$  the temperature at the measurement tray in degrees K. As can be seen, using this method involves measuring the temperature as well as the pressure on the measurement tray. For a multicomponent mixture solving Eqs. (11) and (11a) would involve an iterative procedure.

The values of the constants are given in Table 3.

Once  $x_m$  is known,  $x_s$  can be calculated from the following equation:

$$x_s = x_m + \left(\frac{\partial x}{\partial S}\right)_m (S - S_m) \quad (12)$$

The derivative  $(\partial x / \partial S)_m$  can be calculated in a number of different ways:

- i) Assume the value is constant, take the average from simulations with the detailed model. It was found that this simple method does not provide good estimates of  $x_s$ , thus it will not be explored further.
- ii) Assume two temperatures are measured, for example,  $T_m$  and  $T_{m+1}$ , then the derivative can be calculated from:

$$\left(\frac{\partial x}{\partial S}\right)_m = \left(\frac{\partial x}{\partial T}\right)_m \left(\frac{\partial T}{\partial S}\right)_m \quad (12a)$$

$$\left(\frac{\partial T}{\partial S}\right)_m = \frac{T_{m+1} - T_m}{S_{m+1} - S_m} \quad (12b)$$

in which  $(\partial x / \partial T)_m$  is assumed to be constant and  $(\partial T / \partial S)_m$  follows from Eq. (8a).

The concentration  $x_s$  could also be calculated directly from the temperature  $T_s$ , using the following equation:

$$x_s = x_{s,\text{ref}} + \left(\frac{\partial x}{\partial T}\right)_s (T_s - T_{s,\text{ref}}) \quad (13)$$

Table 3  
Values of constants in Eqs. (10) and (11)

$A(1)$	−4342.35
$A(2)$	−4798.58
$B(1)$	17.97036
$B(2)$	18.1490
$(\partial x / \partial T)_m$	−0.039
$x_{m,\text{ref}}$	0.505
$T_{m,\text{ref}}$	68.010
$p$ at steady state	124.11 mmHg

in which the derivative is assumed to be constant. The values of the derivatives and the reference values are, as before, obtained from simulations with the detailed tray to tray model.

The values of the constants for Eqs. (12) and (13) are given in Table 4.

#### 4. Inferential models

Two other models were developed in order to develop a control strategy for the tower overhead composition (i) a PLS estimator for the profile position and (ii) a PLS estimator for the overhead composition.

Since in a situation where the overhead composition is controlled, the column will not move far away from its steady state operating region, a PI temperature controller on tray 25 was installed, manipulating the reflux.

This controller was loosely tuned and subsequently the column was subjected to feed flow and feed composition changes. Temperatures, pressure and flows as well as profile position and column overhead composition were acquired from the detailed model.

From practical operating experience with binary distillation columns it is known that from measurements with two or more temperature sensors it is possible to estimate the overhead composition accurately and that one does not need to include more process variables in the estimation. Therefore, the inferential models for the profile position and overhead concentration were built using one, two and three temperature sensors. The following criterion was used for the Root Mean Square Error of Prediction (RMSEP):

$$\text{RMSEP} = \sqrt{\frac{\sum_{i=1}^N (y(i) - \hat{y}(i))^2}{N}} \quad (14)$$

Training data consisted of a series of changes in feed flow rate and feed composition with a training set size of 3000 data points. The two best models for the estimation of the profile position using one, two and three sensors are given in Table 5.

As can be seen, the case with measurements from three sensors gives the lowest error.

Table 4  
Values of constants in Eqs. (12) and (13)

$S$	0.84806
$S_m$	0.83333
$(\partial x / \partial S)_m$	4.438
$(\partial x / \partial T)_m$	−0.039 °C
$(\partial x / \partial T)_s$	−0.031 °C
$x_{s,\text{ref}}$	0.570
$T_{s,\text{ref}}$	65.91 °C

Table 5

Linear PLS models for profile position using one, two and three temperature measurements

Temperature measurement on tray	RMSEP
21	$2.81E-3$
22	$3.67E-3$
4, 27	$7.12E-4$
5, 27	$7.41E-4$
16, 20, 24	$8.10E-4$
4, 25, 26	$5.37E-4$

Table 6

Linear PLS model for overhead concentration, using one, two and three temperature measurements

Temperature measurement on tray	RMSEP
27	$8.29E-3$
22	$2.10E-4$
4, 26	$3.07E-4$
4, 27	$4.75E-5$
16, 20, 24	$9.30E-4$
4, 25, 26	$4.57E-5$

Table 6 shows the six best performing PLS models for estimating the overhead composition, based on one, two and three temperature measurements.

From a PCA analysis it was found that the variations in the temperatures on trays 4 and 27 explained more than 95% of the variation in the data set. In addition, even though the RMSEP values may be different, the estimated profile position and estimated concentration hardly improves going from two to three temperature measurements. Therefore, the temperatures on trays 4 and 27 were used in the PLS models for the profile position and overhead concentration. The following linear static inferential model was found for estimating the position of the concentration profile inflection point:

$$S_{\text{LPLS}} = a_1 T_4 + b_1 T_{27} + c_1 \quad (15)$$

Since a linear PLS model for estimation of the profile position performed moderately (see next section), also a nonlinear PLS model was developed using a nonlinear inner relationship as explained in Wold, Kettaneh-Wold and Skageberg (1989). The following equation for calculation of the scores was used:

$$t = a_2 T_4 + b_2 T_{27} + c_2 \quad (16)$$

and the following nonlinear equation for calculation of the profile position:

$$S_{\text{NLPLS}} = a_3 t^2 + b_3 t + c_3 \quad (17)$$

For the overhead composition (high purity) the following static inferential model was found:

$$\ln(1 - x_{D,\text{PLS}}) = a_4 T_4 + b_4 T_{27} + c_4 \quad (18)$$

Table 7

Parameters for inferential models

$a_1$	$-2.20615E-2$	$a_3$	$+2.522181E-3$
$b_1$	$+9.11350E-3$	$b_3$	$1.474268E-2$
$c_1$	$+2.5998734$	$c_3$	$0.8475674$
$a_2$	$-0.22500267$	$a_4$	$-0.10909475$
$b_2$	$+0.97435641$	$b_4$	$+0.50266475$
$c_2$	$-34.193794$	$c_4$	$-23.601935$

The parameter values of all models are given in Table 7.

It is interesting to note that Luyben (1982) gives the following method to determine the most sensitive temperature along the column. For the types of disturbances expected (feed flow changes and composition changes) calculate the matrix shown in Eq. (19), where 0 refers to the bottom tray and 30 to the top tray.

$$K_{32 \times 2} = \begin{bmatrix} \frac{\partial T_0}{\partial F} & \frac{\partial T_0}{\partial z_F} \\ \dots & \dots \\ \frac{\partial T_i}{\partial F} & \frac{\partial T_i}{\partial z_F} \\ \dots & \dots \\ \frac{\partial T_{30}}{\partial F} & \frac{\partial T_{30}}{\partial z_F} \end{bmatrix} \quad (19)$$

$$K = U \Sigma V^T \quad (20)$$

This gain matrix is not suitable when two or more tray temperatures have to be found. To decrease the interaction of the sensor locations, Luyben suggests the Singular Value Decomposition as a solution. The gain matrix  $K$  is then decomposed into the unique component matrices, as shown in Eq. (20), in which

$K$ , the  $31 \times 2$  gain matrix;

$U$ , a  $31 \times 2$  column orthogonal matrix, the columns are called the left singular vectors;

$V$ , a  $2 \times 2$  matrix, the columns are called the right singular matrix;

$\Sigma$ , a  $2 \times 2$  diagonal matrix with scalars, that are called the singular values.

Matrices  $U$  and  $K$  are a measure of the sensor sensitivity. The elements of the  $U$  matrix can be plotted against the tray number and the maximum absolute values are an indication of the most sensitive tray temperature locations. It was found that for this binary system, the most sensitive tray locations were 10 and 25, whereas the PCA analysis indicated that the best temperature locations were trays 4 and 27. This is most likely due to the fact that the PLS estimator not only takes into account the highest sensitivity of the tray temperature to feed flow and feed composition changes, but also the sensitivity of the temperature difference to these changes, as can be seen from the modified Eq. (18)



$$\ln(1 - x_{D,PLS}) - c_4 = (a_4 + b_4)T_{27} + a_4(T_4 - T_{27}) \quad (21)$$

## 5. Model predictions

The developed models for estimation of  $T_s$  were tested against the detailed model in order to verify how well they predict. Step disturbances were introduced in the feed rate of  $\pm 5\%$  and in the feed composition of  $\pm 15\%$ . The model predictions using one temperature measurement (Eq. (9)) and two temperature measurements (Eq. (8)) are shown in Fig. 4. It can be seen that both models predict well. The prediction using two temperatures coincides with the interpolated value of the temperature, the prediction using one temperature is also good.

For the estimation of  $x_s$  the following cases were compared:

Case 1: Eqs. (10) and (12).

Case 2: Eqs. (11) and (12).

Case 3: Eqs. (9) and (13).

Fig. 5 compares the estimated values of  $x_s$  with values from the detailed model. As can be seen, there is not much difference between cases one and three, they deviate slightly from the true values, whereas case two coincides with the true values of  $x_s$  but it is also the more elaborate method in which the temperature and pressure have to be measured. This method is only attractive for binary systems since the computation of concentration from temperature and pressure in multi-component systems would involve an iterative calculation, which is not attractive when the inferential measurement is used in a control loop.

For the linear PLS estimator the prediction of the profile position is compared against the profile position from the detailed model. The result is shown in Fig. 6 for feed changes and feed composition changes.

As can be seen the prediction is not very good. The initial part of the response is good, and this is the most

important part for control. To improve the prediction of the profile position, a nonlinear PLS model was developed. The performance is shown in Fig. 7; it can be concluded that the prediction capabilities have been significantly improved.

For the PLS overhead concentration estimator, the concentration is compared against the overhead concentration from the detailed model and the result for both types of disturbances is shown in Fig. 8. Also in this case, the prediction is good.

Shin et al. (2000) used a similar nonlinear wave model estimator in a Generic Model control strategy. Even though they performed their study on a simulated column, no plots were shown of the performance of the profile position estimation by means of the wave model. The nonlinear wave model presented in this investigation shows some interesting differences with the previously mentioned study. Firstly, Shin et al. relate the average flows in one section of the column to the flows in the other column section by the following equations:

$$\bar{L} = L + qF$$

$$V = \bar{V} + (1 - q)F \quad (22)$$

where  $q$  is the liquid mole fraction of the key component in the feed. In our study we found that liquid and vapor flows in both column sections are very much affected by the feed flow rate and feed composition changes. Especially the effect of the latter type of disturbances are not very well represented by Eq. (22). Therefore, the method presented in this paper (Eqs. (4) and (5)) are better suited for estimating the liquid and vapor flow, respectively.

Another difference with Shin's investigation is that Shin uses Eq. (8) to calculate the temperature on the measurement tray by assuming that  $T_s$  can be computed from a  $T_{xy}$  diagram of the system. In our study we are dealing with a distillation under low pressure and the temperature on the representative tray is also dependent on the absolute pressure, which is not measured on that tray. Therefore, the temperature on the measurement tray is used to calculate  $T_s$  instead. It can be concluded that the model presented in this study is much simpler than the model presented by Shin et al. and is, therefore, more attractive from an application point of view.

Kano et al. (2000) recently performed a study in which dynamic PLS was used to predict the compositions in an alcohol–water–ether distillation column. The authors found that five column temperatures, the reflux flow rate, the reboiler duty and the reboiler pressure should all be used to make acceptable predictions of the compositions. In this study only one composition was estimated and the column is a binary column. It was found that two temperatures gave already an adequate prediction of the composition and adding a third temperature only gave marginal improve-

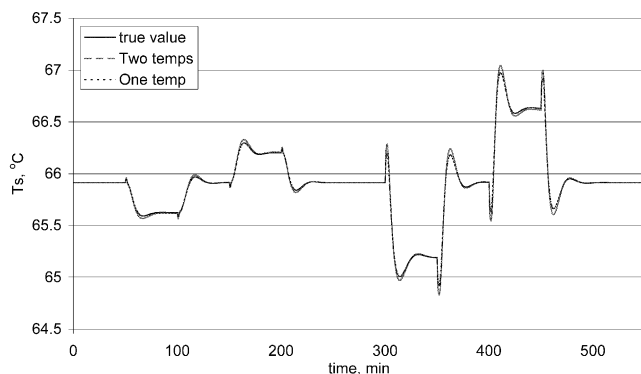


Fig. 4. Estimation of temperature at representative tray using one (Eq. (8)) and two temperature measurements (Eq. (9)).

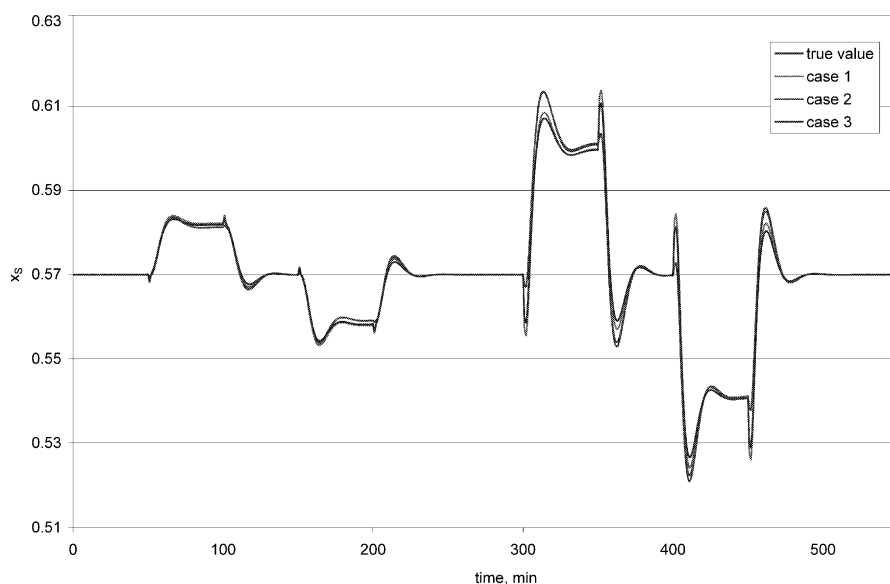


Fig. 5. Estimation of composition at representative tray using different methods.

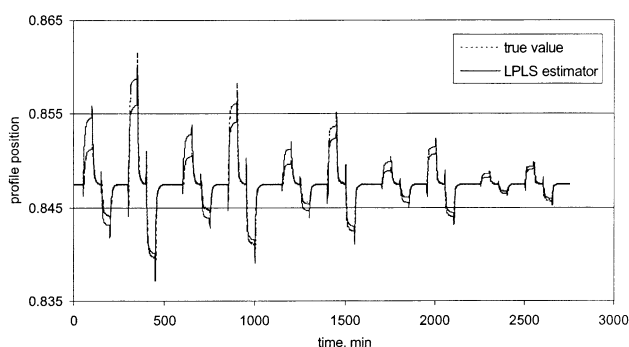


Fig. 6. Estimation of profile position at representative tray for feed flow rate and feed composition changes using linear PLS.

ment. Also addition of other variables such as the reflux flow rate, the reboiler duty and the reboiler pressure gave only marginal improvements.

## 6. Control study

The purpose of the modeling work is to use the model in a control strategy in which ultimately the overhead composition of the column is controlled. It is assumed that the true overhead composition can be measured with a dead time of 10 min.

When a model is used and an inferential variable is controlled (slave controller), a second feedback control loop is required to adjust the setpoint of the inferential control loop in order to avoid offset in the controlled variable (master controller). The setpoint of the inner control loop depends on the inferential model that is used. In the case where the inferential model is the nonlinear wave model,  $u_{\Delta}$  is the model output and it is assumed that control should be such that  $u_{\Delta}$  is maintained at zero. In case of PLS model-based control, the profile position is the model output and it should be

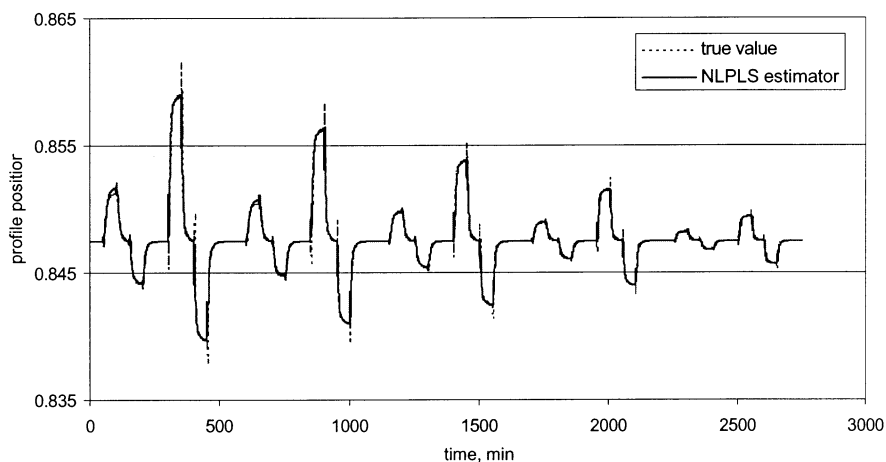


Fig. 7. Estimation of profile position at representative tray for feed flow rate and feed composition changes using nonlinear PLS.

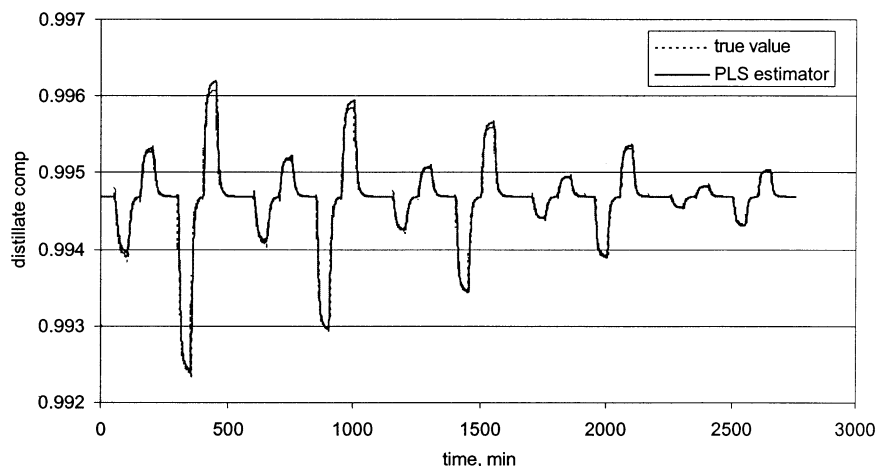


Fig. 8. Estimation of overhead composition for feed flow rate and feed composition changes using PLS.

maintained at a preset target. When the PLS based composition controller is used, the composition should be maintained at a preset target. In all cases the reflux is the manipulated variable.

The settings of the inner and outer loop PI controllers are determined by a search algorithm, such that the integrated total sum of the absolute error (ITAE) is minimal. The PI algorithm used is the discrete standard velocity type algorithm.

The following cases were investigated:

- a, non-linear wave model with Eqs. (3), (8), (10) and (12);
- b, non-linear wave model with Eqs. (3), (8), (11) and (12);
- c, non-linear wave model with Eqs. (3), (9) and (13);
- d, non-linear PLS model for profile position, Eqs. (16) and (17);
- e, non-linear PLS model for concentration, Eq. (18);
- f, control using a single temperature measurement (on tray 25).

Fig. 9 shows the typical response of the overhead composition for some of the control configurations when only a slave controller is active. A step disturbance in the feed composition of +30% was given (twice the

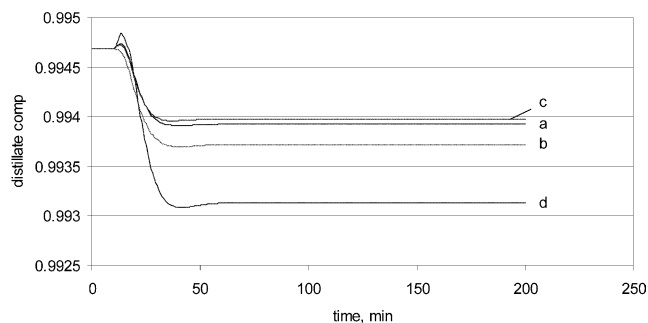


Fig. 9. Transient behavior of distillate composition for a feed composition change of +30%, using different slave controllers.

magnitude of the disturbance used for PLS model training). As can be seen there is some remaining offset in the overhead composition and a master controller is required to eliminate this.

The closed loop response of different control systems is shown in Fig. 10 for a step change in the feed flow rate of +10% (also twice magnitude of the disturbance used for PLS model training).

It can be seen that all model-based controllers perform well. The PI controllers using the nonlinear PLS estimation of the profile position and top concentration, respectively (d, e), perform marginally better than the PI controllers using the profile position from the nonlinear wave model as measured variable. Control using a single tray temperature does not perform as well as control using inferential models for the profile position and overhead composition, but compared with feedback control of the overhead composition only, it performs acceptably. The maximum deviation from setpoint in case of control using a single temperature is  $-0.00094$ , whereas control using feedback of the measured composition only results in a maximum deviation of  $-0.01769$  for a feed change of +10%.

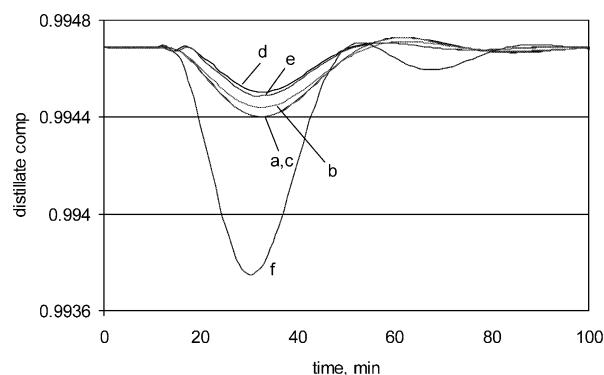


Fig. 10. Distillate composition in case of cascade control for a step disturbance in the feed rate of +10%.

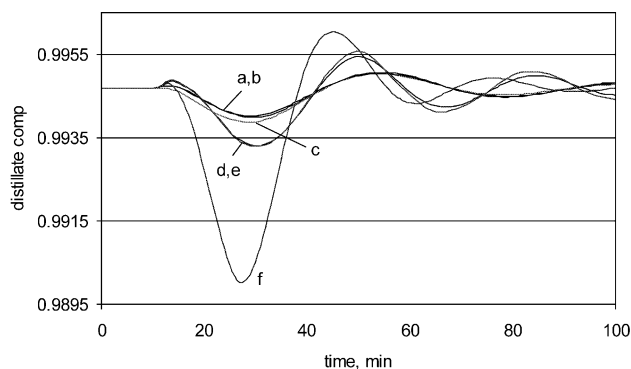


Fig. 11. Distillate composition in case of cascade control for a step disturbance in the feed composition of +30%.

Fig. 11 shows control of the overhead composition using the same control strategies as before but now for a step disturbance in the feed composition of +10%. A similar pattern is shown as in Fig. 10, the control strategies using inferential measurements for profile position or concentration outperform control using a single tray temperature. In this case the nonlinear wave model is the best performer (a, b, c), and the control strategies using the nonlinear profile position estimator and concentration estimator perform slightly less favorable.

The control strategies were also tested for smaller and larger disturbances, the feed flow rate change varied between  $\pm 1$  and 15% and the overhead composition change varied between  $\pm 1$  and 30%. In all cases responses were similar to the responses shown in Figs. 10 and 11.

Compared with true overhead composition control only, all control strategies e–f perform well and provide a large reduction in maximum deviation from setpoint of the controlled overhead composition. Inferential control using profile position or overhead composition estimation performs better than inferential control using a single temperature measurement.

As can be seen, nonlinear PLS estimators can be developed that perform equally well when applied in a model-based control strategy as a control strategy in which the nonlinear wave model is applied.

The linear PLS estimator for the profile position was not considered in the control strategies. The control strategy that included this estimator performed well for feed composition changes but performed poorly for feed rate changes and disturbances larger than the ones used for training the PLS estimator. This can be expected since the estimation of the profile position is poor. The process-model mismatch was too large in most cases and in closed loop control this lead easily to oscillation in the controlled output.

## 7. Conclusion

In this study the nonlinear wave model was revisited and a number of modifications were proposed. These included proper estimation of the vapor and liquid flow from a mass and enthalpy balance across the tail end of the column. Simple equations for the estimation of the concentration and temperature on the representative tray based on one temperature measurement, two temperature measurements and measurements that included temperature as well as pressure were proposed and compared.

It was shown that a nonlinear profile position estimator and a nonlinear composition estimator could easily be derived from process data obtained from simulations with the detailed model.

Using the inferential measurements from either the nonlinear wave model or from nonlinear PLS models in a cascade control structure, provided the benefit of improved response of the controlled composition. It was also shown that the performance of a control structure based on use of the nonlinear wave model was very similar to the performance of a control structure in which one of the nonlinear PLS models were used.

The linear PLS estimator for the profile position could not be used in a control structure due to poor prediction properties. The nonlinear PLS estimators performed well, even for disturbances that were twice as large as the disturbances used for training the estimator.

In all cases control structures using the nonlinear wave model or nonlinear PLS estimators outperformed a control structure in which a single tray temperature was used as an inferential variable. Using one tray temperature is insufficient to guarantee a constant top quality.

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